

**A NEW MIXED-HYBRID FINITE ELEMENT
METHOD FOR CONVECTION-DIFFUSION PROBLEMS**

A. Serghini Mounim

Department of Mathematics and Statistics

University of Moncton

Moncton, N.-B., E1A 3E9, CANADA

Abstract: In this paper we propose a mixed hybrid finite element method for solving convection-diffusion problems in one space dimension. The method combines a framework of mixed methods, and finite volume philosophy. We derive a new formulation of the convection-diffusion problem in which the general flux is introduced as new variable, and the local conservation is achieved, using the procedure, which consists to impose the continuity conditions of the general flux by means of a Lagrange multiplier. The practicality of the approach relies on a choice of local basis, presented here for the functional discrete subspace of the conserved quantity, consequently, the stabilizing mechanism is intrinsically contained in the trial finite element space. The choice of shape functions is inspired by the problem structure. One of the advantages of the scheme is the upwinding introduced by the basis functions, unlike the usual hat functions, which give a centered schemes. Furthermore, we show particularly its relationship with the most popular scheme for semiconductor problems, in the circumstances, the Scharfetter and Gummel scheme [39]. We also perform some numerical tests, showing the advantages of the scheme.

AMS Subject Classification: 73V05, 76M10, 65L60, 65M60

Key Words: mixed hybrid finite element method, finite volume scheme, convection-diffusion problems

1. Introduction

The convection-diffusion problems are of great practical importance since they appear in many areas, in fluid mechanics, astrophysics, groundwater flow, semi-conductors, etc. and have attracted a lot of attention in recent years.

It is well-known that the classical numerical approaches, such as central finite difference methods and conventional finite element approximations (the classical finite elements basically correspond to centered schemes) do not produce satisfactory approximations to the solution of the dominated convection problems. An effective way of controlling the process of formation of spurious numerical oscillations consists in using appropriate schemes, which try to combine numerical stability with minimal artificial diffusion.

With this aim in view, the discretization via the finite volume methods, is especially efficient, allowing one to easily treat convective terms. There exists a large literature about the finite volume methods; we mention, for example, the family of high resolute schemes, the total variation diminishing method (TVD) [18], flux corrected transport (FCT) methods [3], [43], piecewise parabolic method (PPM) [14], and the essentially non-oscillatory (ENO), (WENO), (CWENO) methods [19], [33], [23], [24].

Alternatively, for the finite element approximation, the stabilization (to avoid the introduction of spurious oscillations) is commonly done via a discontinuous Galerkin (DG) approximation (used, as a variant of Finite Volume), or by using a Streamline-Upwind Petrov-Galerkin (SUPG) method and its variants, e.g. the Galerkin Least Squares (GaLS) method introduced by Hughes and coworkers ([9], [20]). The (DG) finite element methods for the numerical solution of partial differential equations, were first introduced in [36], their stability and convergence analysis was carried out in [27].

More recent numerical methods for the advection diffusion problem are, among others, the Residual-free Bubbles FEM (see e.g. [8]), or the methods proposed in [15], [16].

The weaknesses of the classical finite element methods to treat the convection-diffusion problems (with a small diffusive terms or major convective terms), justify the efforts to develop the methods using the good features of volume schemes to treat the convective terms, as well as the advantages of the mixed finite elements. These advantages are among others, local conservation property, good approximation of the flux variable, versatility and flexibility of the mixed finite element method to deal with the complexity of the geometry or the behavior of the solution, and also their superiority from a theoretical point of view (since a standard framework and large number of results are available

for carrying out their analysis).

In this work, we propose an efficient finite-volume approach, which takes advantage of both methods. This can be achieved by introducing the general flux as new auxiliary and independent variable. To realize the local conservation, Lagrange multipliers on interior nodes were exploited to relax the continuity of functions in the the flux space. The main ingredient in the construction of the scheme is the choice of functional discrete space of the conserved quantity. The basis functions of this space, depends strongly on the convection-diffusion equations, giving one weighted scheme. Hence, the weights are the key ingredient of the scheme, and are built to fit the physic parameters.

To our knowledge, this is the first scheme built in the framework of mixed methods with such a choice of trial finite element space. In particular, this enables us to show in a natural way, the relationship between our scheme and the famous Scharfetter-Gummel scheme [39] (the so-called exponential fitting method) see also [2], and independently described by [1] and [21].

The outline of this paper is as follows, in the next section we present the general theory that is used to derive the abstract formulation. In Section 3, we introduce the evolution mixed and hybrid finite-volume scheme. The link with the Scharfetter and Gummel flux as well as the relationship between our basis functions choice and the standard hat functions are given. The analogy with the finite volume methods is given in Section 4. Finally, in the last section numerical tests are presented.

2. The Abstract Formulation

In this section, we introduce the abstract formulation for the convection-diffusion problem. The methodology uses the framework of mixed hybrid finite element methods.

Our model problem is find $u : I \times]0, T[\rightarrow \mathbb{R}$ such that

$$\begin{cases} \frac{\partial u}{\partial t} - \nu \frac{\partial^2 u}{\partial x^2} + \beta \frac{\partial u}{\partial x} = 0, & \text{in } I \times]0, T[, \\ u(x, 0) = u_0(x), & x \in I, \\ u(c) = \gamma(t) \quad \text{and} \quad u(d) = \delta(t). \end{cases} \quad (1)$$

Here $I =]c, d[$, the velocity is $\beta \in \mathbb{R}$, the diffusion coefficient is $\nu > 0$, and $u = u(x, t)$ is a conserved quantity.

It is known that the basic idea of mixed methods is to introduce, together with the solution u of (1), an auxiliary and independent variable, in our case we

introduce $P = F(u)$ as new unknown, where $F(u) = -\nu \frac{\partial u}{\partial x} + \beta u$, represents the general flux, composed from convection and diffusion fluxes. Consequently, the mixed variational form of the problem (1) reads as follows:

$$\frac{\partial u}{\partial t} + \frac{\partial P}{\partial x} = 0, \quad \text{in } I \times]0, T[,$$

with given initial data $u(x, 0) = u_0(x)$, and corresponding suitable boundary conditions.

In order to define the hybridization of the mixed formulation, we need some additional notations. Let a partition of I into a finite element $I_i = \{x \mid x_i < x < x_{i+1}\}$, possibly irregular mesh, with nodes $x_0 = c < x_1 < \dots < x_N = d$, and use the notation of the mesh size $h_i = x_{i+1} - x_i$, $0 \leq i \leq N - 1$. Furthermore, we consider the spaces, $M_2 = \{\mu : \{x_0, x_1, \dots, x_N\} \rightarrow \mathbb{R}\}$, $\overline{M}_2 = \{\mu \in M_2 \mid \mu_0 = \mu_N = 0\}$, $M_1 = L^2(I)$, $X_1 = H^1(I)$ and $X_2 = \{q \in M_1, q|_{I_i} \in H^1(I_i)\}$.

Next we relax the continuity of P across interelement boundaries with a Lagrange multiplier λ and this latter becomes *additional* unknown of the problem. Indeed, we have:

$$\begin{aligned} \sum_i \int_{I_i} P(t) q \, dx &= \sum_i \int_{I_i} F(u(t)) q \, dx \\ &+ \sum_i (\lambda_{i+1}(t) q(x_{i+1}^-) - \lambda_i(t) q(x_i^+)), \quad \forall q \in X_2. \end{aligned}$$

From this last relation, we then obtain the conservation of the general flux in each cell, enforcing the continuity of the flux in a weak form by a Lagrange multiplier technique:

$$\sum_i (P(x_i^+, t) - P(x_i^-, t)) \mu = 0, \quad \forall \mu \in \overline{M}_2.$$

This equation implies the weak continuity of P at the nodes, where $P(x_i^\pm)$ are the correspondent left and right traces of P at x_i .

Hence, the problem can also be formulated in the following form: given $T > 0$, $u_0 \in L^2(I)$, and corresponding suitable boundary conditions, for almost

every $t \in]0, T[$, find $(u(t), \lambda(t)) \in X_1 \times M_2$, and $P(t) \in X_2$ such that:

$$\left\{ \begin{array}{l} \frac{d}{dt}(u(t), v) + b(P(t), v) = 0, \quad \forall v \in M_1, \\ a(P(t), q) = a(F(u), q) + \sum_i (\lambda_{i+1}(t)q(x_{i+1}^-) - \lambda_i(t)q(x_i^+)), \\ \sum_i (P(x_i^+, t) - P(x_i^-, t))\mu = 0, \quad \forall \mu \in \overline{M}_2, \end{array} \right. \quad \forall q \in X_2, \quad (2)$$

we denote by $(., .)$ the scalar product in $L^2(I)$, $b(q, v) = \sum_i \int_{I_i} \frac{dq}{dx} v dx$, and

$$a(p, q) = \sum_i \int_{I_i} pq dx.$$

The above form requires less smoothness to define the solution u that one imposed (in fact, it is sufficient to have $u(t) \in L^2(I)$ and $F(u)|_{I_i} \in L^2(I_i)$), the reason for this choice will be clear in the next section.

The techniques used in the forthcoming sections are similar to [15], [16].

3. Spatial Approximation

In order to construct the approximation of our formulation, and since, $P(t) \in X_2$ and $\lambda(t) \in M_2$, the standard choice of functional discrete spaces is $M_{1h} \subset M_1$, $X_{2h} \subset X_2$ and $M_{2h} \subset M_2$, the test and trial finite element spaces are defined as,

$$M_{1h} = \{ v_h \in L^2(I); v_h|_{]x_i, x_{i+1}[} \in \mathbb{P}_0, \quad 0 \leq i \leq N - 1 \},$$

$$X_{2h} = \{ q_h \in X_2; q_h|_{]x_i, x_{i+1}[} \in \mathbb{P}_1, \quad 0 \leq i \leq N - 1 \},$$

$$M_{2h} = \{ \mu_h : \{x_0, x_1, \dots, x_N\} \rightarrow \mathbb{R} \}, (= M_2),$$

where \mathbb{P}_k denotes the space of all polynomials on I_i of degree k , ($k = 0, 1$).

We now introduce a last trial finite element space $X_{1h} \neq M_{1h}$ (Petrov-Galerkin formulation type), which will be used in our discrete formulation. Let $\omega_{j+1/2} \in H^1(I) (\subset C^0(I))$, be a function with compact support and $0 \leq \omega_{j+1/2}(x) \leq 1, \forall x \in I$, and let $X_{1h} = \{\omega_{j+1/2}\}$ denote some suitable finite dimensional subspace of $H^1(I)$. Suppose also that $\{\omega_{1/2}, \omega_{3/2}, \dots, \omega_{N-1/2}\}$ is basis for X_{1h} . The procedure, and a natural way for choosing a class of shape functions will be described further.

We can now give the discrete problem of (2). Given $T > 0$, $u_0 \in L^2(I)$, and corresponding suitable boundary conditions, for almost every $t \in]0, T[$, find $(u_h(t), \lambda(t)) \in X_{1h} \times M_{2h}$, and $P_h(t) \in X_{2h}$ such that:

$$\left\{ \begin{array}{l} \frac{d}{dt}(u_h(t), v_h) + b(P_h(t), v_h) = 0, \quad \forall v_h \in M_{1h}, \\ a(P_h(t), q_h) = a(F(u_h), q_h) + \sum_i (\lambda_{i+1}(t)q_h(x_{i+1}^-) - \lambda_i(t)q_h(x_i^+)), \\ \sum_i (P_h(x_i^+, t) - P_h(x_i^-, t))\mu = 0, \quad \forall \mu \in \overline{M}_{2h}, \end{array} \right. \quad \forall q_h \in X_{2h}, \quad (3)$$

for given $u_h(0) = u_0 \in L^2(I)$, and each grid function $(u_{i+1/2})_{0 \leq i \leq N-1}$ is identified with the finite element function $u_h(x)$ belonging to the conforming space X_{1h} , i.e.

$$u_h(x, t) = \sum_{i=0}^{N-1} c_{i+1/2}(t)\omega_{i+1/2}(x).$$

Note that, the variable P_h can be eliminated a priori at the element level, leading to a final algebraic system in the variables $u_h(t)$ and $\lambda(t)$ only.

The basic idea of our approach is the choice of $\omega_{i+1/2}$, and their use to construct u_h , hence, they play a fundamental role in our approach. The selection of these shape functions depends strongly on the equation that we have to resolve, and is also motivated physically.

In fact, it seems intuitively reasonable to consider the basis functions $\omega_{j+1/2}$ in each sub-interval $I_{i+1/2} =]x_{i+1/2}, x_{i+3/2}[$ to be solution of the local problem

$$\mathbf{L}u = 0,$$

subject to the boundary conditions $\omega_{j+1/2}(x_{i+1/2}) = \delta_{ji}$, $0 \leq i, j \leq N-1$ and where $\mathbf{L} := -\nu \frac{d^2}{dx^2} + \beta \frac{d}{dx}$ (of course, this choice is not unique but is efficient).

It follows

$$\omega_{i+1/2}(x) = \begin{cases} \frac{\exp(p_{i-1/2}(x - x_{i-1/2})/h_{i-1/2}) - 1}{\exp(p_{i-1/2}) - 1}, & x \in I_{i-1/2} \\ 1 - \frac{\exp(p_{i+1/2}(x - x_{i+1/2})/h_{i+1/2}) - 1}{\exp(p_{i+1/2}) - 1}, & x \in I_{i+1/2} \end{cases}$$

where $h_{i+1/2} = (h_{i+1} + h_i)/2$, and $p_{i+1/2} = \frac{\beta h_{i+1/2}}{\nu}$ being the local ‘‘Peclet’’ number.

Let us define $\omega(x; p) = \frac{\exp(px)-1}{\exp(p)-1}$, the weight function, which verifies in particular $\omega(0; p) = 0$ and $\omega(1; p) = 1$. Therefore, the expression of the shape functions becomes

$$\omega_{i+1/2}(x) = \begin{cases} \omega\left(\frac{x - x_{i-1/2}}{h_{i-1/2}}; p_{i-1/2}\right), & x \in I_{i-1/2}, \\ 1 - \omega\left(\frac{x - x_{i+1/2}}{h_{i+1/2}}; p_{i+1/2}\right), & x \in I_{i+1/2}. \end{cases}$$

It is clear that all above properties of $\omega_{i+1/2}$ are respected, notice particularly, the fact that $0 \leq \omega_{i+1/2}(x) \leq 1, \forall x \in I_{i-1/2} \cup I_{i+1/2}$, follows from the maximum principle. And, we have also $u_h(x, t)|_{[x_{i-1/2}, x_{i+1/2}]} = u_{i-1/2}(t) + (u_{i+1/2}(t) - u_{i-1/2}(t))\omega_{i+1/2}(x)$, with $u_{i+1/2}(t) = c_{i+1/2}(t)$.

From the expression of the basis functions, we conclude

$$F(\omega_{i+1/2})(x) = \begin{cases} -\beta \frac{\exp(p_{i-1/2}(x - x_{i-1/2})/h_{i-1/2})}{\exp(p_{i-1/2}) - 1} + \beta\omega_{i+1/2}(x), & x \in I_{i-1/2} \\ \beta \frac{\exp(p_{i+1/2}(x - x_{i+1/2})/h_{i+1/2})}{\exp(p_{i+1/2}) - 1} + \beta\omega_{i+1/2}(x), & x \in I_{i+1/2}. \end{cases}$$

Notice also that $(F(\omega_{i-1/2}) + F(\omega_{i+1/2}))|_{I_{i-1/2}} = \beta$.

We next determine the terms

$$F(u_h)|_{I_i} = \tilde{F}_i(t) + \tilde{F}_{i+1}(t), \tag{4}$$

with

$$\begin{aligned} \tilde{F}_i(t) &= \tilde{F}(x_i, t) \\ &= u_{i-1/2}(t)F(\omega_{i-1/2})|_{I_{i-1/2}} + u_{i+1/2}(t)F(\omega_{i+1/2})|_{I_{i-1/2}}. \end{aligned} \tag{5}$$

Moreover, \tilde{F}_i can be interpreted as a fluxes at the boundaries x_i (see below for more explicit expression), and the $F(\omega_{i+1/2})$ play the role of an upwinding weights. Indeed, alone contain so much information, they depend not only of h , but also of the ‘‘Peclet’’ number $p_{i+1/2}$, and for $\beta > 0$, $(\omega_{i-1/2})|_{x_i, x_{i+1/2}[}$ has more ‘‘weight’’ than $(\omega_{i+1/2})|_{x_i, x_{i+1/2}[}$. They have the merit to deal with problems, where there is substantial variation of the ‘‘Peclet’’ number. Consequently, the stabilizing mechanism is intrinsically contained in the trial finite element space X_{1h} .

As known, it is hard to determine an appropriate parameter of upwinding, that introduces just enough dissipation to preserve monotonicity without causing unnecessary smearing. One of our goals, is to derive a scheme with adapting weights to physic parameters.

Furthermore, the expression of F can be rewritten as

$$F(\omega_{i+1/2})(x) = \begin{cases} -\frac{\nu}{h_{i-1/2}}B(p_{i-1/2}), & x \in I_{i-1/2}, \\ \frac{\nu}{h_{i+1/2}}B(-p_{i+1/2}), & x \in I_{i+1/2}. \end{cases} \quad (6)$$

$B(x)$ stands for the Bernoulli function, defined for any $x \in \mathbb{R}$ as

$$B(x) = \begin{cases} \frac{x}{e^x - 1}, & \text{if } x \neq 0, \\ 1, & \text{otherwise.} \end{cases}$$

On the other hand, the association of (3), (4) and (5), and a direct computation, yield the approximate flux P_h in each I_i

$$P_h(x, t) = \alpha(t) + \gamma(t)(x - x_{i+\frac{1}{2}}), \quad (7)$$

where

$$\alpha(t) = \frac{\lambda_{i+1}(t) - \lambda_i(t)}{h_i} + \frac{1}{2}(\tilde{F}_{i+1}(t) + \tilde{F}_i(t)),$$

and

$$\gamma(t) = 6\frac{(\lambda_{i+1}(t) + \lambda_i(t))}{h_i^2} + \frac{1}{2h_i}(\tilde{F}_{i+1}(t) - \tilde{F}_i(t)).$$

Using some elementary algebra, it is easy to obtain in each sub-interval I_i , the semi-discrete scheme

$$\begin{cases} \frac{d}{dt}u_{i+1/2}(t) + 6\frac{(\lambda_{i+1}(t) + \lambda_i(t))}{h_i^2} + \frac{1}{2h_i}(\tilde{F}_{i+1}(t) - \tilde{F}_i(t)) = 0, \\ \frac{1}{h_{i-1}}\lambda_{i-1}(t) + (\frac{2}{h_{i-1}} + \frac{2}{h_i})\lambda_i(t) + \frac{1}{h_i}\lambda_{i+1}(t) \\ \qquad \qquad \qquad = \frac{1}{8}(\tilde{F}_{i+1}(t) - \tilde{F}_{i-1}(t)). \end{cases} \quad (8)$$

The midpoint rule have been used to approximate the integral $\int_{I_i} u_h(t) dx$. For simplicity's sake, we assume an uniform grid, thus an examination of the second equation of the above system, reveals that the Lagrange multiplier λ insuring the weak continuity of the general flux, can be interpreted as the coefficients of the B splines interpolant the function $G(x, t) = \frac{h}{8}(\tilde{F}(x+h, t) - \tilde{F}(x-h, t))$.

Moreover, the above scheme can be generalized immediately to deal with the source term, and $\beta(x, t)$ (i.e. $\beta \neq \text{const}$). More precisely, assuming for example that the velocity is piecewise constant on each sub-interval of I (i.e. $\beta_i(t) = \beta|_{I_{i-1/2}}$), or identifying each grid function

$$(\beta_{i+1/2}(t))_{0 \leq i \leq N-1},$$

with the finite element function $\beta_h(x, t) = \sum_{i=0}^{N-1} \beta_{i+1/2}(t) \varphi_{i+1/2}(x)$, where $\varphi_{i+1/2}$ are the usual hat functions (if β is assumed liner in each $I_{i+1/2}$).

Next, we try to show the link between the standard basis functions and the ones constructed here. First, note that $|\beta(x - x_{i+1/2})|/\nu \leq |\beta h|/\nu$ for all $x \in I_{i+1/2}$, where $h = \max_i h_{i+1/2}$ $0 \leq i \leq N - 1$, and if it is assumed that $|\beta h|/\nu \rightarrow 0$ (i.e. $|\beta h| \ll \nu$), then $\omega_{i+1/2} \rightarrow \varphi_{i+1/2}$, with

$$\varphi_{i+1/2}(x) = \begin{cases} \frac{x - x_{i-1/2}}{h_{i-1/2}}, & x \in I_{i-1/2}, \\ 1 - \frac{x - x_{i+1/2}}{h_{i+1/2}}, & x \in I_{i+1/2}, \end{cases}$$

is the standard hat function for the i th node (the shape functions $\varphi_{i+1/2}$ and $\omega_{i+1/2}$ are shown in the figure below, see Figure 1). More generally, we give below the relation between the hat and the shape functions.

$$\omega_{i+1/2}(x) = \begin{cases} \omega(\varphi_{i+1/2}(x); p_{i-1/2}), & x \in I_{i-1/2}, \\ 1 - \omega(1 - \varphi_{i+1/2}(x); p_{i+1/2}), & x \in I_{i+1/2}. \end{cases}$$

Finally, we have $\int_{x_{i-1/2}}^{x_{i+3/2}} \varphi_{i+1/2}(x) dx = \int_{x_{i-1/2}}^{x_{i+3/2}} \omega_{i+1/2}(x) dx = h$, for the uniform mesh.

Remark 1. Notice also that $B(-x) = e^x B(x) = x + B(x)$, and it is well-known in semiconductor device simulation that the Bernoulli function has to be implemented very carefully for numerical computations. It can be suggested to implement it as follows:

$$B(x) = \begin{cases} 0, & \text{for } |x| > M \text{ and } x > 0, \\ -x, & \text{for } |x| > M \text{ and } x < 0, \\ 1 - \frac{x}{2} \left(1 + \frac{x}{6}\right) \left(1 - \frac{x^2}{60}\right), & \text{for } |x| < \epsilon. \end{cases}$$

Here, $M = 80$ and $\epsilon = 10^{-4}$.

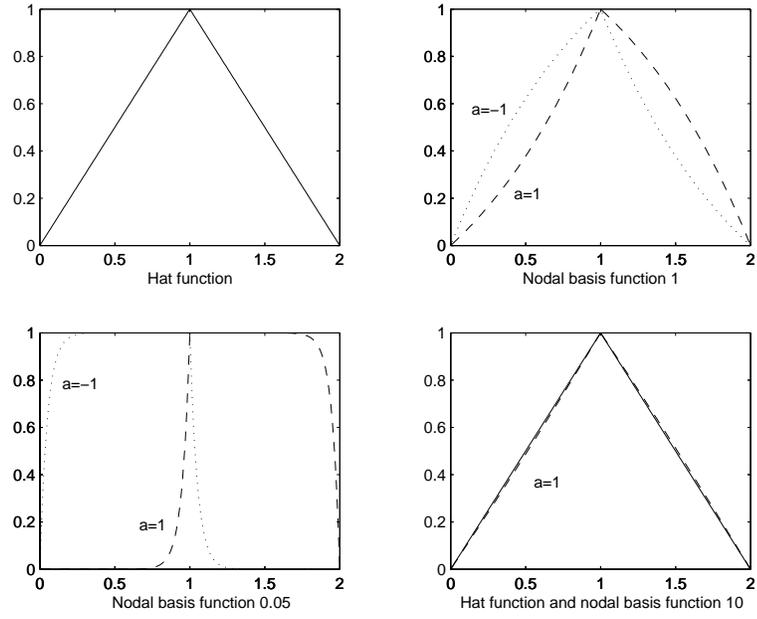


Figure 1: Basis functions: $\varphi_{i+1/2}$ with $h = 1$, and $\omega_{i+1/2}$ with $h = 1$, and the velocity $a = \pm 1$, the diffusion coefficient is $\nu = 1, 0.05, 10$, resp.

Furthermore, thanks to (5) associated to (6) we can exhibit the expression of \tilde{F}_i by

$$\tilde{F}_i(t) = \frac{\nu}{h_{i-1/2}}B(-p_{i-1/2})u_{i-1/2}(t) - \frac{\nu}{h_{i-1/2}}B(p_{i-1/2})u_{i+1/2}(t), \quad (9)$$

this numerical flux is nothing else than the celebrated Scharfetter and Gummel (S.G.) flux [39] (see also [1] and [21]), and the resulting scheme has a very important property of monotonicity and local conservation. In 1969, the (S.G.) scheme have been first suggested for the numerical solution for convection dominated problems of semiconductor and gaz discharge plasmas. It has been derived “heuristically”, where F_i , $u_{i+1/2}$, ν , $\beta = \mu E$, denote respectively the current density at the cell boundary (physical notation J_i), the electron number density (physical notation n_i), the diffusion coefficient, the mobility (μ) and the electric field strength (E).

This link has been already established by means of an exponential fitting mixed (EFM) finite element method. The EFM finite element method introduced for the drift-diffusion continuity equation (we refer to [5], [6], [7] and [32]), can be summarized as follows:

1. Transformation of the problem using the Slotboom variable to a symmetric form.
2. Discretization of the form obtained by mean of the mixed finite element method.
3. In order to go back to the original unknown, a suitable discrete version of the inverse transform of (1) is used.

The properties of the Bernoulli function enable us to write

$$\tilde{F}_i(t) = \frac{u_{i-1/2}(t) \max(\beta, 0) - u_{i+1/2}(t) \max(-\beta, 0)}{-\nu B(|p_{i-1/2}|) \frac{u_{i+1/2}(t) - u_{i-1/2}(t)}{h_{i-1/2}}}, \quad (10)$$

observe the contribution of convective and diffusive fluxes in the expression of the general flux, depends on $B(|p_{i-1/2}|)$. Finally, instead of using the Bernoulli function, and starting from $B(x) \simeq 1 - \frac{x}{2} - \frac{x^2}{12} + \frac{x^3}{120} + \frac{x^4}{720}$, if $|x| < \epsilon$, we can recover in the standard way, for example the upwind scheme (if we use $B(|x|) \simeq 1$), the centered scheme (setting $B(|x|) \simeq 1 - \frac{|x|}{2}$).

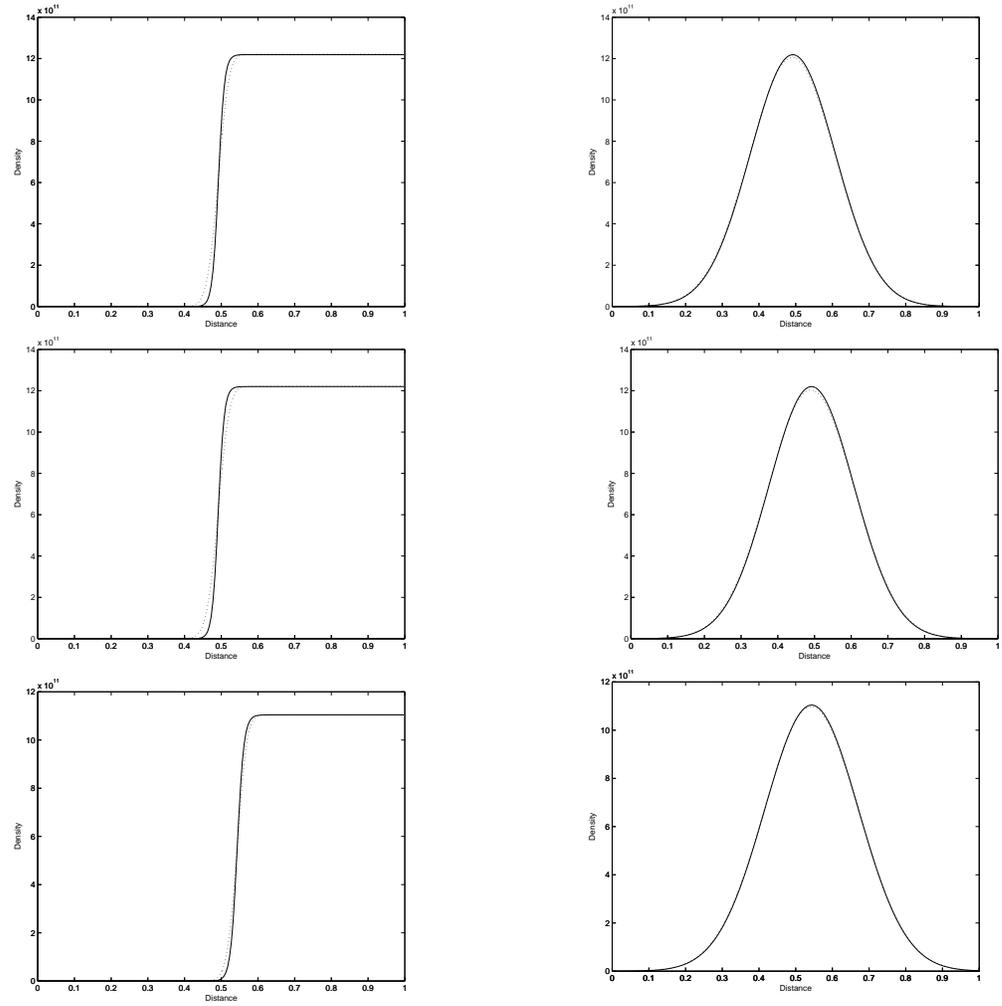


Figure 2: The structure of “shock wave” profile. Gaussian profile transport. Exact solution —, and numerical solution ···

4. Relationship with Finite Volume Methods

In this section, we show how the finite volume schemes can be derived from a dual mixed and hybrid finite element method. For this purpose, we use trapezoidal quadrature formula to approximate the integral $\int_{I_i} l_j l_k dx$ (coefficients of the mass matrix, l_i are the shape functions), yielding a diagonal matrix which has the advantage of uncouple the equations as we will see further. First, let us recall the equations which allow us to exhibit the expression of the numerical scheme;

$$\left\{ \begin{array}{l} \int_{I_i} \frac{du_h(t)}{dt} v_h dx + \int_{I_i} \frac{dP_h(t)}{dx} v_h dx = 0, \\ \int_{I_i} P_h(t) q_h dx = \int_{I_i} F(u_h) q_h dx + (\lambda_{i+1}(t) q_h(x_{i+1}^-) - \lambda_i(t) q_h(x_i^+)). \end{array} \right. \quad (11)$$

To these equations are added the continuity condition. If we use trapezoidal quadrature formula, and analogously to above, one gets:

$$\left\{ \begin{array}{l} \frac{d}{dt} u_{i+1/2}(t) + 2 \frac{(\lambda_{i+1}(t) + \lambda_i(t))}{h_i^2} + \frac{(\tilde{F}_{i+1}(t) - \tilde{F}_i(t))}{2h_i} = 0, \\ \lambda_i(t) = \frac{h_i h_{i-1}}{h_i + h_{i-1}} \frac{(\tilde{F}_{i+1}(t) - \tilde{F}_{i-1}(t))}{8}, \end{array} \right. \quad (12)$$

or

$$\left\{ \begin{array}{l} \frac{d}{dt} u_{i+1/2}(t) + 2 \frac{\lambda_{i+1}(t) + \lambda_i(t)}{h_i^2} + \frac{1}{2} \frac{\tilde{F}_{i+1}(t) - \tilde{F}_i(t)}{h_i} = 0, \\ 2 \frac{\lambda_{i+1}(t) + \lambda_i(t)}{h_i^2} = \frac{1}{4} \left(\frac{h_{i-1}}{h_i} \frac{\tilde{F}_{i+1}(t) - \tilde{F}_{i-1}(t)}{h_i + h_{i-1}} + \frac{h_{i+1}}{h_i} \frac{\tilde{F}_{i+2}(t) - \tilde{F}_i(t)}{h_{i+1} + h_i} \right). \end{array} \right.$$

Thus, the numerical general flux (7) expressed at the interface cells of I_i and I_{i-1} , reduces to a convex combination of Sharfetter-Gummel flux:

$$P_h(x_i, t) = \frac{h_{i-1} \tilde{F}_{i-1}(t) + 3(h_{i-1} + h_i) \tilde{F}_i(t) + h_i \tilde{F}_{i+1}(t)}{4(h_i + h_{i-1})}. \quad (13)$$

Note that the elimination of Lagrange multiplier λ , implies lack of smoothing in the resulted volume scheme.

For an uniform mesh the expression above gives

$$P_h(x_i, t) = \frac{\tilde{F}_{i-1}(t) + 6\tilde{F}_i(t) + \tilde{F}_{i+1}(t)}{8}, \quad (14)$$

or with the help of (10), the general numerical flux can be split into two parts

$$P_h(x_i, t) = C_i(t) - \nu B(|p|) D_i(t), \quad (15)$$

where

$$C_i(t) = \max(\beta, 0) \frac{u_{i-3/2}(t) + 6u_{i-1/2}(t) + u_{i+1/2}(t)}{8} - \max(-\beta, 0) \frac{u_{i-1/2}(t) + 6u_{i+1/2}(t) + u_{i+3/2}(t)}{8},$$

and

$$D_i(t) = \frac{5}{8} \frac{u_{i+1/2}(t) - u_{i-1/2}(t)}{h} + \frac{3}{8} \frac{u_{i+3/2}(t) - u_{i-3/2}(t)}{3h}.$$

Firstly, observe that D_i is a convex combinations of two centered approximations of $\frac{\partial u}{\partial x}$. Moreover, the scheme which is constructed to deal with the convection-dominated equations, is able to reproduce a pure-diffusive regime, i.e. $\beta = 0$.

Secondly, for simplicity we suppose $\beta > 0$, and we deduce

$$C_i(t) = \beta \frac{u_{i-1/2}(t) + u_{i+1/2}(t)}{2} - \frac{\beta}{2} \left(\frac{3u_{i+1/2}(t) - 2u_{i-1/2}(t) - u_{i-3/2}(t)}{4} \right). \quad (16)$$

To analyze the limit behavior of (15) as $\nu \rightarrow 0$ and h fixed. Note that if $\nu \ll |p|$ (i.e. $B(p) \rightarrow 0$), the numerical general flux tends to convective flux (16). Remark that C_i is composed from the average of the values in cells on either side of each edge, augmented by appropriate dissipative terms

$$\frac{3u_{i+1/2}(t) - 2u_{i-1/2}(t) - u_{i-3/2}(t)}{4}.$$

This last expression can be interpreted as a flux which approximates $h \frac{\partial u}{\partial x}$, comparatively with the dissipative terms $(u_{i+1/2}(t) - u_{i-1/2}(t))$ of the (S.G.) convective flux C_i^{SG} (for high Peclet numbers the (S.G.) scheme degenerates into the standard Engquist-Osher scheme).

Before to give some numerical results, it should be noted that the above scheme can be extended to multidimensional cases. The details about this extension will be reported in another paper.

5. Numerical Results

We conclude this paper with some numerical examples, illustrating the efficiency of the scheme. Consider the convection-diffusion equation

$$\frac{\partial u}{\partial t} - \nu \frac{\partial^2 u}{\partial x^2} + \frac{\partial(\beta u)}{\partial x} = 0, \tag{17}$$

here u denotes the electron number density, the electric field $\beta(x, t) = -10^4 x$, $x \in [0, 1]$, and the diffusion coefficient $\nu = 1$. With the above parameters, (17) is a advection-dominated problem, hence the exact solution of the pure convection equation is given by $u(x, t) = u_0(xe^{-10^4 t})e^{-10^4 t}$, u_0 is the initial condition. In our tests we take firstly the model of the shock wave

$$u_0(x) = \gamma + \frac{\delta}{2} \left\{ 1 + \tanh\left(\frac{x - x_0}{\sigma_1}\right) \right\}, \tag{18}$$

secondly the Gaussian profile

$$u_0(x) = \gamma + \delta \exp\left(-\frac{(x - x_0)^2}{\sigma_2}\right), \tag{19}$$

where the parameters $\sigma_1 = 0.02$, $\sigma_2 = 0.04$, $\gamma = 10^2$ and $\delta = 10^{12}$.

We present the results obtained using the numerical general flux P_h (15), and considering a piecewise constant approximation of the velocity $\beta_h(x) \simeq \beta(x)$ of the form $\beta_h(x) = \sum_{j=1}^{N-1} \beta_j \mathbb{1}_{]x_{j-1/2}, x_{j+1/2}[}$. For the time discretization we used the first-order accurate Euler explicit scheme, $\frac{u_{i+1/2}^{n+1} - u_{i+1/2}^n}{\Delta t} + \frac{P_{i+1}^n - P_i^n}{h_i} = 0$, $u_{i+1/2}^n = u_h(x_{i+1/2}, n\Delta t)$, $P_i^n = P_h(x_i, n\Delta t)$ and Δt denotes the temporal step size. The exact solution (of the “pure” advective equation) and the results of numerical experiments with the initial solution (18) (resp. (19)) are summarized in Figure 2.1 ((a), (c), (e)) (resp. Figure 2.2 (b), (d), (f)). On the figures below, the physical and numerical coefficients are chosen to be those given in the table below:

Figure	Courant number	cells	time steps
(a), (b)	0.4	200	100
(c), (d)	0.2	200	200
(e), (f)	0.2	200	100

As planned, the depicted results are similar to results obtained by the standard (S.G.) scheme. Moreover, we conclude that the proposed method does not suffer from extensive numerical dispersion or nonphysical oscillations, which is the

main drawback of standard finite element methods when used for convection-dominated problems.

Finally, we conclude that in this work, we have explored a mixed-hybrid finite element framework with an original process for the choice of the trial finite element space. This approach enabled us to derive a weighted scheme, capable to deal with problems where there is substantial variation of the Peclet number. It is well-known that this is a weakness of the conventional finite element approximations. Moreover, the construction of the scheme is simple, its link with the popular (S.G.) scheme is established. On the other hand, the numerical experiments show its property of monotonicity.

References

- [1] D.N. Allen, R.V. Southwell, Relaxation methods applied to determine the motion, in 2D of a viscous fluid past a fixed cylinder, *Quart. J. Mech. Appl. Math.*, **8** (1955), 129-145.
- [2] R.E. Bank, D.J. Rose, W Fichtner, Numerical methods for semiconductor device simulation, *SIAM J. Sci. Stat.*, **4** (1983), 493-514.
- [3] J.P. Boris, L.D. Brook, Flux corrected transport, SHASTA, a fluid transport algorithm that works, *J. Comput. Phys.*, **11** (1973), 38-69.
- [4] F. Brezzi, M. Fortin, *Mixed and Hybrid Finite Element Methods*, Springer Series in Computational Mathematics, Springer-Verlag (1991).
- [5] F. Brezzi, L. Marini, P. Pietra, Méthodes d'éléments finis mixtes et schémas de Scharfetter-Gummel, *C.R. Acad. Sci. Paris*, **305** (1987), 599-604.
- [6] F. Brezzi, L. Marini, P. Pietra, Numerical simulation of semiconductor devices, *Comp. Meth. Appl. Mech. Engrg.*, **75** (1989), 493-514.
- [7] F. Brezzi, L. Marini, P. Pietra, Two-dimensional exponential fitting and applications to drift-diffusion models, *SIAM J. Num. Anal.*, **26** (1989), 1342-1355.
- [8] F. Brezzi, Russo, Choosing bubbles for advection-diffusion problems, *Math. Models Methods Appl. Sci.*, **4** (1994), 571-587.
- [9] A.N. Brooks, T.J.R. Hughes, Streamline upwind/Petrov-Galerkin formulations for convection dominated flows with particular emphasis on the

- incompressible Navier-Stokes equations, *Comput. Methods Appl. Mech. Mech. Engrg.*, **32** (1982), 199-259; In: *FENOMECH'81*, Part 1, Stuttgart (1981).
- [10] P.G. Ciarlet, *The Finite Element Method for Elliptic Problems*, North-Holland (1978).
- [11] B. Cockburn, S. Hou, C.W. Shu, TVB Runge-Kutta local projection P^1 -discontinuous Galerkin finite element method for conservation laws 4: The multi-dimensional case, *Math. Comp.*, **54** (1990), 545-581.
- [12] B. Cockburn, S.Y. Lin, C.W. Shu, TVB Runge-Kutta local projection P^1 -discontinuous Galerkin finite element method for conservation laws 3: One-dimensional systems, *J. Comput. Phys.*, **84** (1989), 90-113.
- [13] B. Cockburn, C.W. Shu, TVB Runge-Kutta local projection P^1 -discontinuous Galerkin finite element method for conservation laws 2: General framework, *Math. Comp.*, **52** (1989), 411-453.
- [14] P. Collela, P.R. Woodward, The piecewise parabolic method (PPM) for gas dynamics simulation, *J. Comput. Phys.*, **54** (1984), 174-201.
- [15] M. Fortin, A. Serghini Mounim, Mixed and hybrid finite element methods for convection-diffusion equations and relationship with finite volume, Part I, *Calcolo*, Submitted.
- [16] M. Fortin, A. Serghini Mounim, Mixed and hybrid finite element methods for convection-diffusion equations and relationship with finite volume, Part II, *Calcolo*, Submitted.
- [17] E. Godlewski, P.A. Raviart, *Hyperbolic Systems of Conservation Laws*, Mathématiques et Applications, Ellipse (1991).
- [18] A. Harten, High-resolution schemes for hyperbolic conservation laws, *J. Comput. Phys.*, **49** (1983), 357-393.
- [19] A. Harten, S. Osher, Uniformly high order accurate nonoscillatory schemes, *SIAM*, **24** (1987), 279-310.
- [20] T.J.R. Hughes, L.P. Franca, G.M. Hulbert, A new finite element formulation for computational fluid dynamics, 8. The Galerkin/least-squares method for advective-diffusive equations, *Comput. Methods Appl. Mech. Engrg.*, **73** (1989), 173-189.

- [21] A.M. Il'in, A difference scheme for a differential equation with a small parameter multiplying the second derivative, *Matematičeskije Zametki*, **6**, No. 2 (1969), 237-248.
- [22] A.A. Kulikovskiy, A more accurate scharfetter-gummel algorithm of electron transport for semiconductor and gas discharge simulation, *Journal of Comput. Phys.*, **119** (1995), 149-155.
- [23] A. Kurganov, D. Levy, A third-order semi-discrete central scheme for conservation laws and convection-diffusion equations, *SIAM Journal on Scientific Computing*, **22**, No. 4, 1461-1488.
- [24] A. Kurganov, E. Tadmor, New high-resolution central schemes for non-linear conservation laws and convection-diffusion equations, *J. Comput. Phys.*, **160** (2000), 214-282.
- [25] R.D. Lazarov, I.D. Mishev, P.S. Vassilevski, Finite volume methods for convection-diffusion problems, *SIAM J. Numer. Anal.*, **33** (1996), 31-55.
- [26] A.Y. Le Roux, *Approximation de Quelques Problèmes non Linéaires*, Université de Rennes, Thèse, Analyse numérique (1979).
- [27] P. Lesaint, P.A. Raviart, On a finite element method for solving the neutron transport equation, In: *Mathematical Aspect of Finite Elements in PDE* (Ed. C de Boor), Academic Press (1974), 89-123.
- [28] R.J. LeVeque, *Numerical Methods for Conservation Laws*, Lectures in Mathematics, Birkhauser (1990).
- [29] R.J. LeVeque, *Finite Volume Methods for Hyperbolic Problems*, Cambridge Texts in Applied Mathematics (2002).
- [30] R.H. MacNeal, An asymmetrical finite difference network, *Q. Appl. Math.*, **11**, 295-310.
- [31] A. Majda, Compressible fluid flow and systems of conservation laws in several space variables, *Bull. Applied Math. Sciences*, **53** Springer-Verlag (1984).
- [32] L. Marini, P. Pietra, New mixed finite element schemes for current continuity equations, *COMPEL*, **9** (1990), 257-268.
- [33] H. Nessyahu, E. Tadmor, Non-oscillatory central differencing for hyperbolic conservation laws, *JCP*, **87**, No. 2 (1990), 408-463.

- [34] S.V. Patankar, *Numerical Heat Transfer and Fluid Flow*, Series in Computational Methods in Mechanics and Thermal Sciences (1980).
- [35] P.A. Raviart, J.M. Thomas, *A Mixed Finite Element Method for 2-nd Order Elliptic Problems*, Lecture Notes in Mathematics, **606**, Springer-Verlag, New-York (1977), 292-315.
- [36] W.H. Reed, T.R. Hill, *Triangular Mesh Methods for the Neutron Transport Equation*, Technical Report, LA-UR-73-479, Los Alamos, Scientific Laboratory (1973).
- [37] P.L. Roe, *Some Contributions to the Modeling of Discontinuous Flows*, Lect. Notes Appl. Math., **22** (1985), 163-193.
- [38] R. Sacco, F. Saleri, Mixed finite volume methods for semiconductor device simulation, *Numer. Methods Partial Differential Equations*, **13** (1997), 215-236.
- [39] D. Scharfetter, H.K. Gummel, Large-signal analysis of a silicon read diode oscillator, *IEEE Trans. Elec. Devices.*, ED-16 (1969), 64-77.
- [40] A. Serghini Mounim, *Méthode d'Éléments Finis Mixtes: Application aux Équations de Convection-Diffusion et Navier-Stokes*, Ph.D. Thesis, Université Laval (2000).
- [41] J. Smoller, *Shock Waves and Reaction-Diffusion Equations*, Spriger-Verlag, Second Edition (1994).
- [42] J.M. Thomas, *Sur L'analyse Numérique des Méthodes d'Éléments Finis Hybrides et Mixtes*, Thèse, Université Pierre et Marie Curie, Paris 6 (1977).
- [43] S.T. Zalasak, Fully multidimensional flux-corrected transport algorithms for fluids, *J. Comput. Phys.*, **31** (1979), 335-362.

